



ELSEVIER

Computer Physics Communications 93 (1996) 322-323

---

---

Computer Physics  
Communications

---

---

## Contents to volume 93

### Computational physics

- Xiao, F., T. Yabe and T. Ito  
Constructing oscillation preventing scheme for advection equation by rational function 1
- Ito, T., H. Eldeib, K. Yoshida, S. Takahashi, T. Yabe and T. Kunugi  
Special-purpose computer for holography HORN-2 13
- Bar-Shalom, A., M. Klapisch and J. Oreg  
Phase-amplitude algorithms for atomic continuum orbitals and radial integrals 21
- Kalkreuter, T. and H. Simma  
An accelerated conjugate gradient algorithm to compute low-lying eigenvalues – a study for the Dirac operator in SU(2) lattice QCD 33
- Schmalian, J., M. Langer, S. Grabowski and K.H. Bennemann  
Self-consistent summation of many-particle diagrams on the real frequency axis and its application to the FLEX approximation 141
- Braun, M., C. Meier and V. Engel  
Nanosecond wave-packet propagation with the Split-Operator Technique 152
- Roy, D., R. Bhattacharya and S. Bhowmick  
Rational approximants using Levin-Weniger transforms 159
- Kramer, K.M. and W.N.G. Hitchon  
Strategies for mesh-handling and model specification within a highly flexible simulation framework 179

### Computer programs in physics

- Grau Carles, A.  
MLOG, the simultaneous standardization of multi-nuclide mixtures 48
- Lamberti, C.  
Interface simulation of strained and non-abrupt III-V quantum wells. Part 1: band profile calculation 53
- Lamberti, C.  
Interface simulation of strained and non-abrupt III-V quantum wells. Part 2: energy level calculation versus experimental data 82
- Montagna, G., O. Nicosini, G. Passarino and F. Piccinini  
TOPAZ0 2.0 - A program for computing de-convoluted and realistic observables around the  $Z^0$  peak 120
- Molisch, A.F., B.P. Oehry, W. Schupita and G. Magerl  
McTrap, a program for the computation of radiation trapping in 3-level atoms including bleaching effects 127



ELSEVIER

Computer Physics Communications 93 (1996) 322-323

---

---

Computer Physics  
Communications

---

---

## Contents to volume 93

### Computational physics

- Xiao, F., T. Yabe and T. Ito  
Constructing oscillation preventing scheme for advection equation by rational function 1
- Ito, T., H. Eldeib, K. Yoshida, S. Takahashi, T. Yabe and T. Kunugi  
Special-purpose computer for holography HORN-2 13
- Bar-Shalom, A., M. Klapisch and J. Oreg  
Phase-amplitude algorithms for atomic continuum orbitals and radial integrals 21
- Kalkreuter, T. and H. Simma  
An accelerated conjugate gradient algorithm to compute low-lying eigenvalues – a study for the Dirac operator in SU(2) lattice QCD 33
- Schmalian, J., M. Langer, S. Grabowski and K.H. Bennemann  
Self-consistent summation of many-particle diagrams on the real frequency axis and its application to the FLEX approximation 141
- Braun, M., C. Meier and V. Engel  
Nanosecond wave-packet propagation with the Split-Operator Technique 152
- Roy, D., R. Bhattacharya and S. Bhowmick  
Rational approximants using Levin-Weniger transforms 159
- Kramer, K.M. and W.N.G. Hitchon  
Strategies for mesh-handling and model specification within a highly flexible simulation framework 179

### Computer programs in physics

- Grau Carles, A.  
MLOG, the simultaneous standardization of multi-nuclide mixtures 48
- Lamberti, C.  
Interface simulation of strained and non-abrupt III-V quantum wells. Part 1: band profile calculation 53
- Lamberti, C.  
Interface simulation of strained and non-abrupt III-V quantum wells. Part 2: energy level calculation versus experimental data 82
- Montagna, G., O. Nicosini, G. Passarino and F. Piccinini  
TOPAZ0 2.0 - A program for computing de-convoluted and realistic observables around the  $Z^0$  peak 120
- Molisch, A.F., B.P. Oehry, W. Schupita and G. Magerl  
McTrap, a program for the computation of radiation trapping in 3-level atoms including bleaching effects 127

Lakshmi Narayan, K.	
Computer modelling of grain microstructure in three dimensions	136
Popelier, P.L.A.	
MORPHY, a program for an automated "atoms in molecules" analysis	212
Judge, R.H., E.D. Womeldorf, R.A. Morris, D.E. Shimp, D.J. Clouthier, D.L. Joo and D.C. Moule	
Computer-assisted analysis of singlet-triplet rotational spectra: application to Case (A), Case (B) and Case (AB) coupling cases in polyatomic molecules	241
Kadlecsik, J.	
Ricci calculus package in REDUCE	265
Ortiz, F. and J.M. Los Arcos	
MCBETH: liquid scintillation counting spectra computation at the dynodic output of the photomultipliers	283
Nguyen, H.V., J.M. Campbell, G.P. Couchell, S. Li, D.J. Pullen, W.A. Schier, E.H. Seabury and S.V. Tipnis	
Programs in C for parameterizing measured $5'' \times 5''$ NaI gamma response functions and unfolding of continuous gamma spectra	289
Louvel, S. and J.-F. Chamayou	
Packing and unpacking histograms with statistical processing	303